Digital twins from microscope image data

James E. McClure ***Virginia Tech National Security Institute*** **16 November 2023**

Digital Twins from microscope image data

Goal — develop computational design platforms that can be used to inform engineering processes and develop mechanisms to control the behavior of small systems

Microscope image data: imaging techniques such as computed micro-tomography and light microscopy can non-invasively resolve the 3D structure of complex materials

AI-based image enhancement: recent advances in artificial intelligence (AI) improve experimental data quality by enhancing signal-to-noise ratio and automate feature labeling

Physics-based models: mesoscale simulations provide a way to understand how the microscopic structure of a system controls the physical responses.

Physics informed machine learning: complex constitutive models can be "learned" from data while imposing physical constraints to accurately capture non-linear processes.

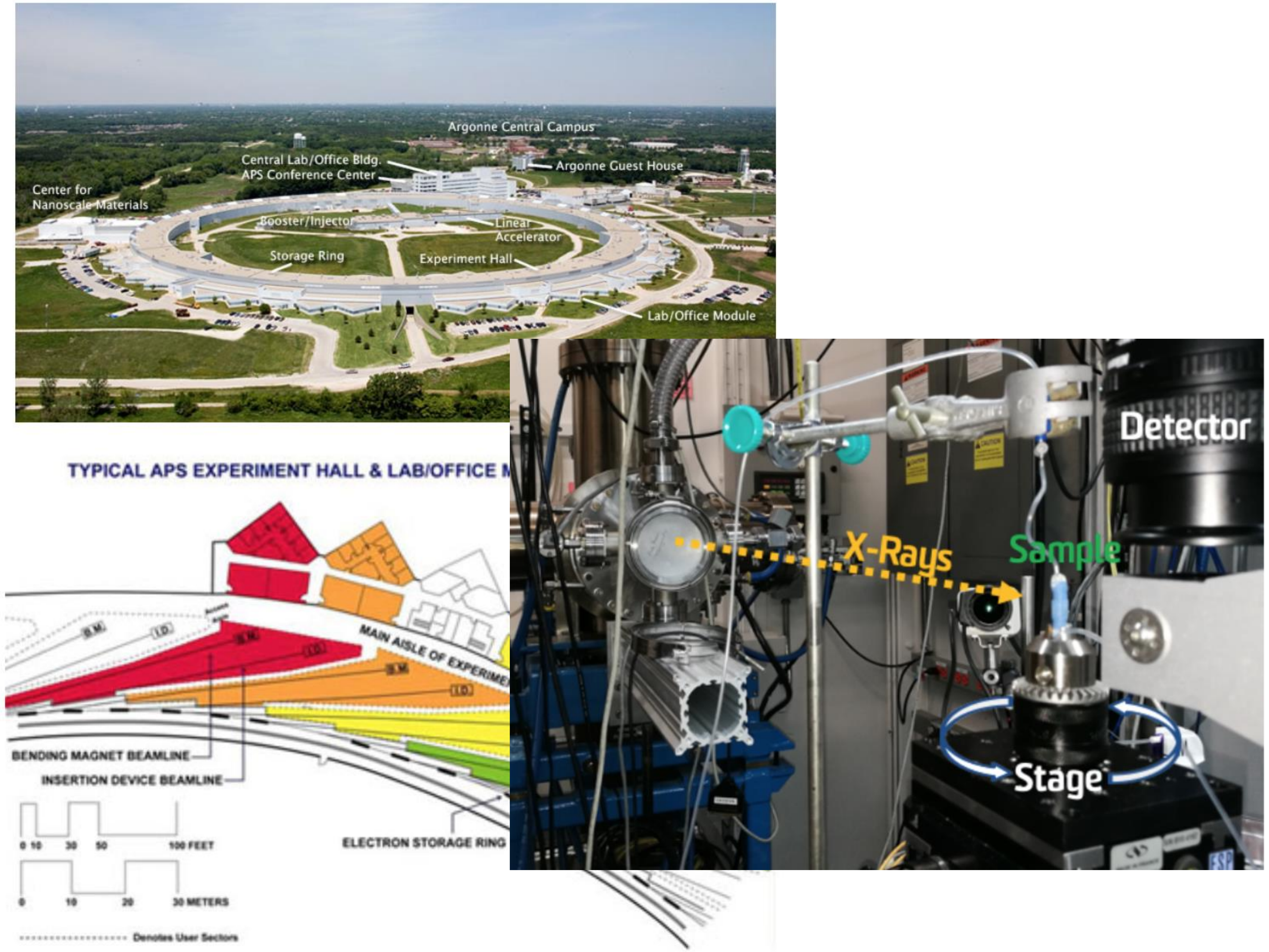
Physics-based data reduction: system responses can be characterized by upscaling simulated behaviors using fundamental physical principles.

Large Data Sources — 3D image data

- Synchrotron light sources are used to carry out a wide range of high-end imaging experiments

- Growth for data generation rates is faster than growth for compute, I/O

- Simulation provides a way to fill in additional physics that are not physically observable



Microscope Image Data

Geologic systems are heterogeous across all scales

- Microscopes provide a basic mechanism to advance understanding for small systems
  - Mineral distribution and microstructure for Mt. Simon sandstone (right)
- Physical behavior at small scales has a deterministic relationship to larger scale behavior
- Fundamental physics are well-understood at small scales

Image Enhancement with AI

- Scientific workflows for microscopy

JE McClure, J Yin, RT Armstrong, KC Maheshwari, S Wilkinson, L Vlcek, Y. da Wang, MA Berrill M Rivers, Toward Real-Time Analysis of Synchrotron Micro-Tomography Data: Accelerating Experimental Workflows with AI and HPC Smoky Mountains Computational Sciences and Engineering Conference, 226-239 (2020) https://doi.org/10.1007/978-3-030-63393-6_15

JE Santos, B Chang, A Gigliotti, E Guiltinan, M Mehana, A Mohan, J McClure, Q Kang, H Viswanathan, N Lubbers, M Prodanovic, M. Pyrc, Learning from a Big Dataset of Digital Rock Simulations, AGU Fall Meeting Abstracts (2021), H25O-1207

- 3D image enhancement, noise reduction and segmentation

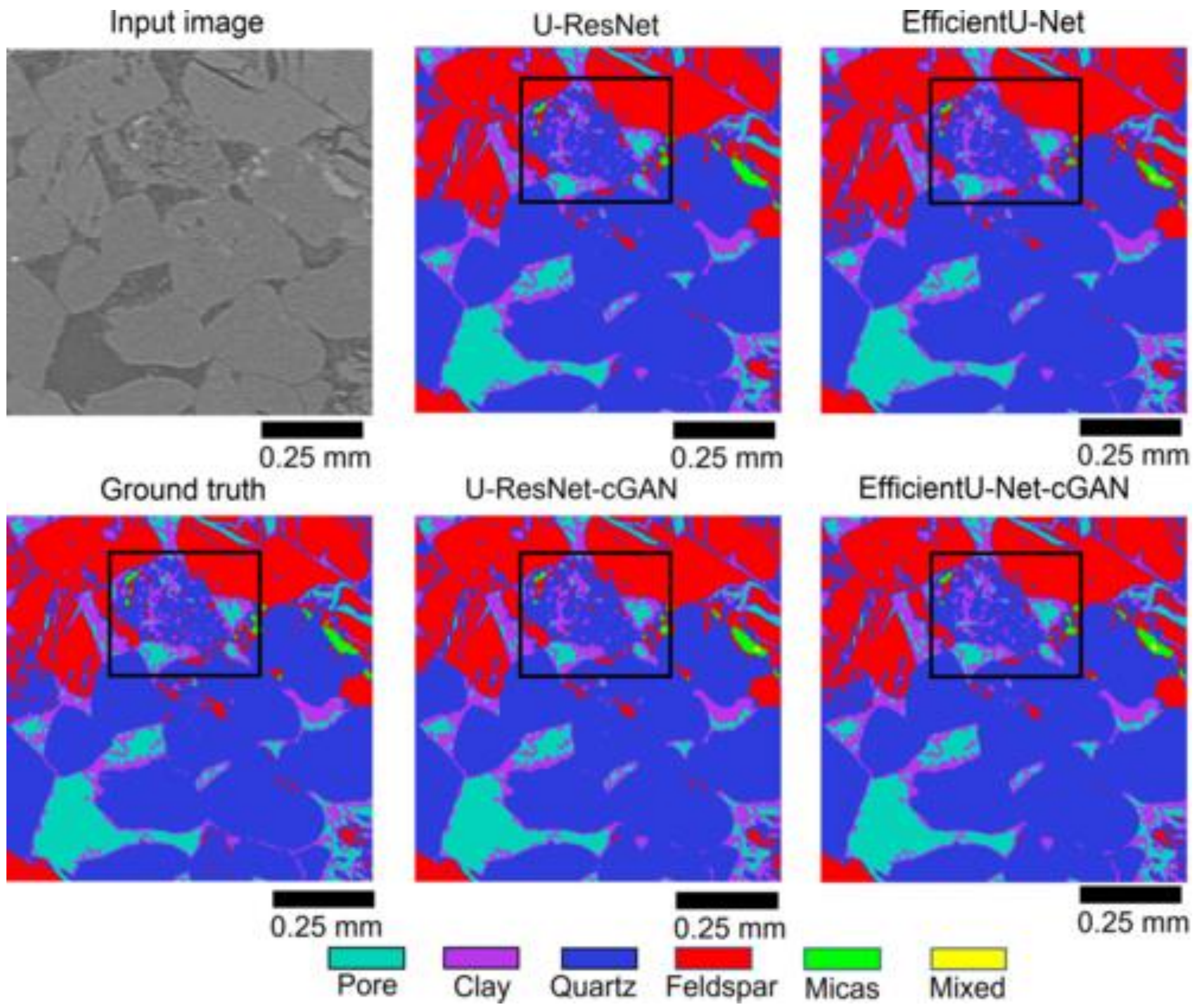
K Tang, Y Da Wang, J McClure, C Chen, P Mostaghimi, RT Armstrong, Generalizable Framework of Unpaired Domain Transfer and Deep Learning for the Processing of Real-Time Synchrotron-Based X-Ray Microcomputed Tomography Images of Complex Structures. *Physical Review Applied* 17 (3), 034048 (2022)

Y Niu, Y Da Wang, P Mostaghimi, JE McClure, J Yin, RT Armstrong, Geometrical-based generative adversarial network to enhance digital rock image quality. *Physical Review Applied* 15 (6), 064033 (2021). https://doi.org/10.1103/PhysRevApplied.15.064033

- Physics-informed machine learning

XH Zhou, JE McClure, C Chen, H Xiao, Neural network–based pore flow field prediction in porous media using super resolution. *Physical Review Fluids* 7 (7), 074302 (2022) https://doi.org/10.1103/PhysRevFluids.7.074302

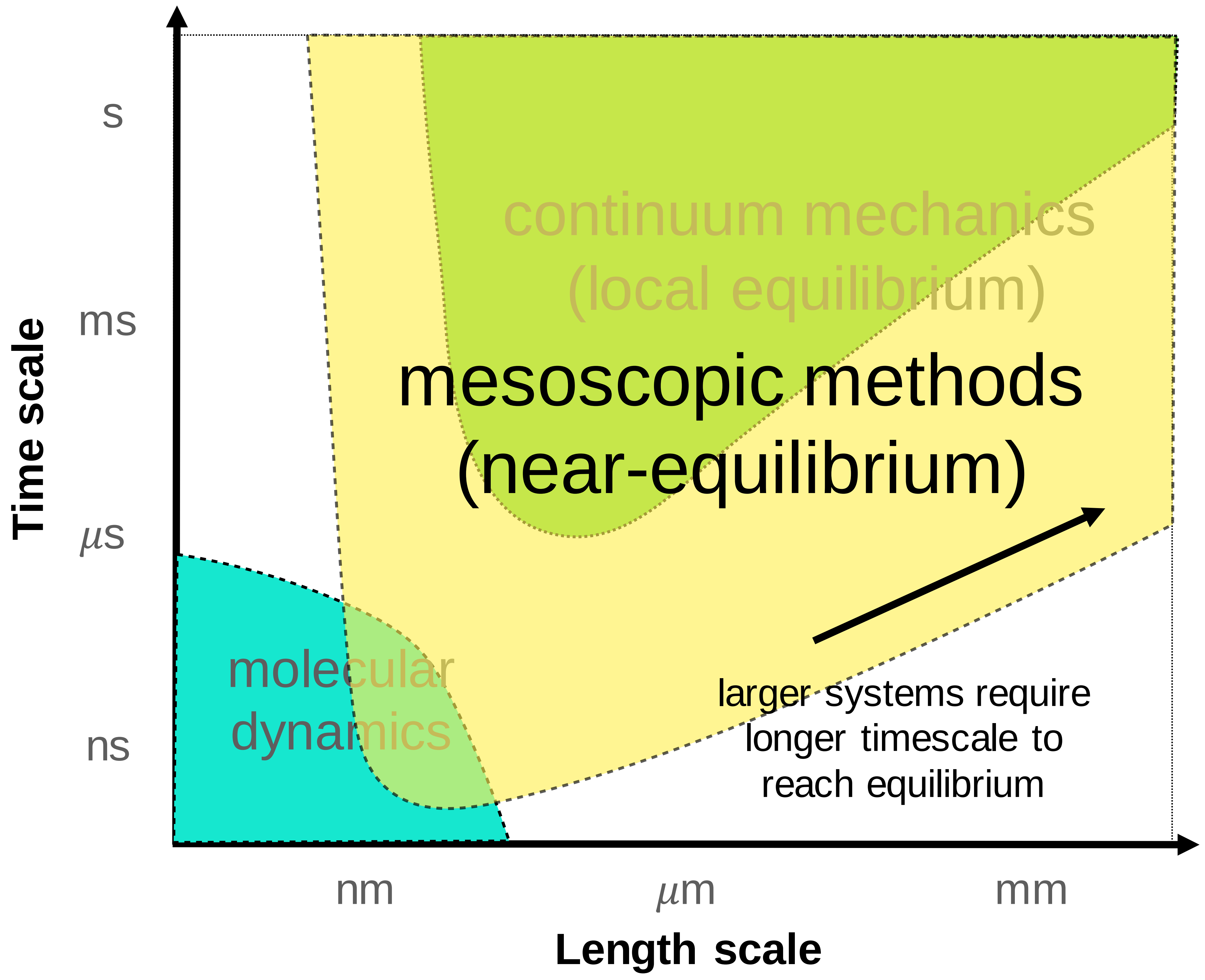
F Alzubaidi, P Mostaghimi, Y Niu, RT Armstrong, G Mohammadi, S Berg, JE McClure Effective permeability of an immiscible fluid in porous media determined from its geometric state. *arXiv:2208.08027*



Physics Simulations

Lattice Boltzmann Methods

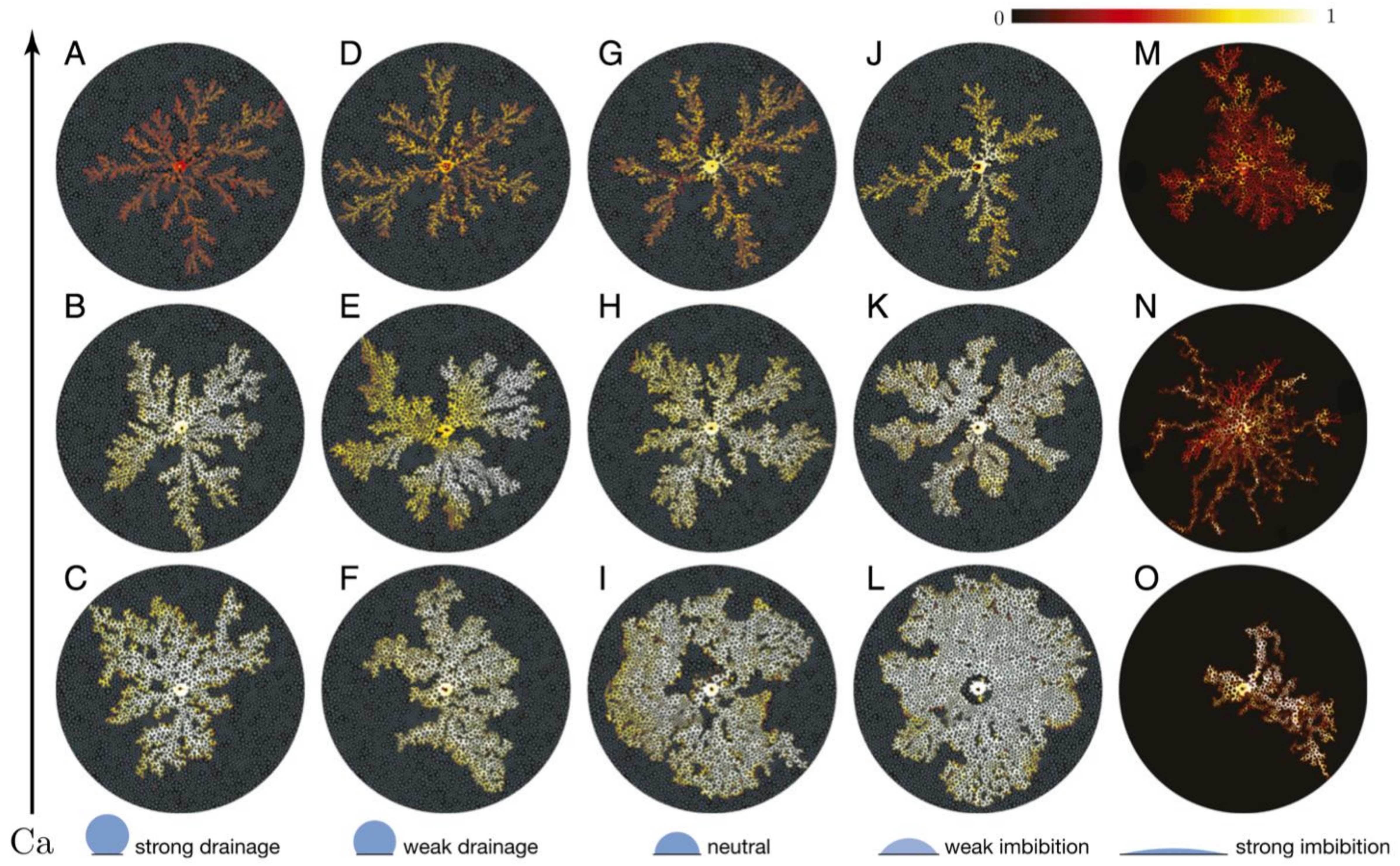
- **Molecular dynamics** — directly resolve molecular trajectories based on Newton's equations of motion
- **Finite element models**— constructed based on continuum mechanical closure approximations
- **Mesoscopic models** — formulated from lower level in modeling hierarchy, rely on coarse grained representation with quasi-molecular closure rules



LBPM

Historical Development

- Applications in water / energy sciences
  - Vadose zone hydrology
  - hydrocarbon recovery
  - CO_2 sequestration
- Fundamental physics questions
  - crossover between viscous / capillary / inertial flow regimes
  - film dynamics



Zhao et al. Comprehensive comparison of pore-scale models for multiphase flow in porous media. *Proceedings of the National Academy of Sciences* (2019), 116 (28) 13799-13806; DOI: 10.1073/pnas.1901619116

LBPM — Scientific Advances

- Geometric explaination of hysteresis for two-fluid flow in porous media

McClure, J.E., Armstrong, R.T., et al. Geometric state function for two-fluid flow in porous media
Phys. Rev. Fluids **3**, 084306 (2018). https://doi.org/10.1103/PhysRevFluids.3.084306

McClure, J.E., Ramstad, T., Li, Z. et al. Modeling Geometric State for Fluids in Porous Media: Evolution of the Euler Characteristic. Transp Porous Med **133**, 229–250 (2020). https://doi.org/10.1007/s11242-020-01420-1

- Time-and-space averaging theory to predict upscaled model forms

McClure, J.E., Berg, S., Armstrong, R.T. Capillary fluctuations and energy dynamics for flow in porous media.
Physics of Fluids **33**, 083323 (2021) (**Featured Article**) https://doi.org/10.1063/5.0057428

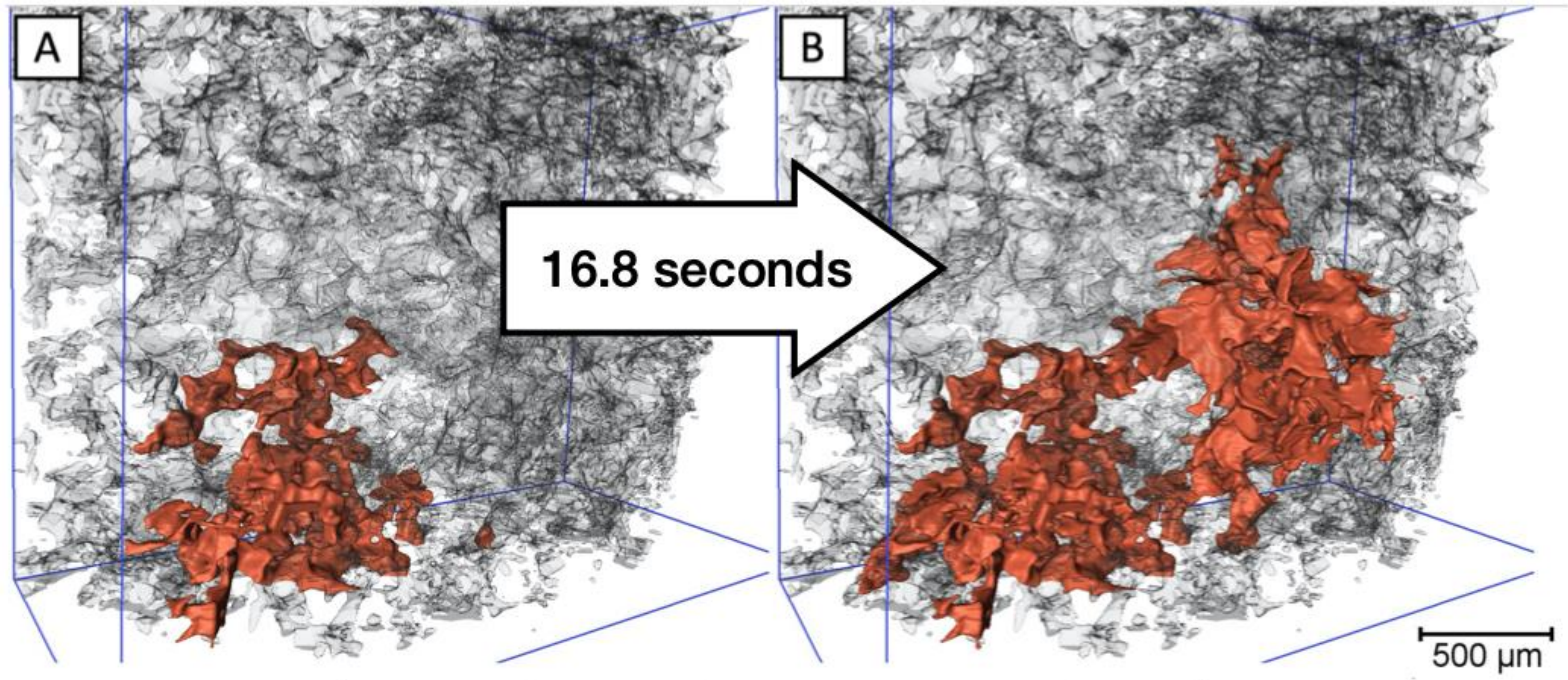
McClure, J.E., Berg, S., Armstrong, R.T. Thermodynamics of fluctuations based on time-and-space averages.
Phys. Rev. E **104**, 035106 (2021) https://doi.org/10.1103/PhysRevE.104.035106

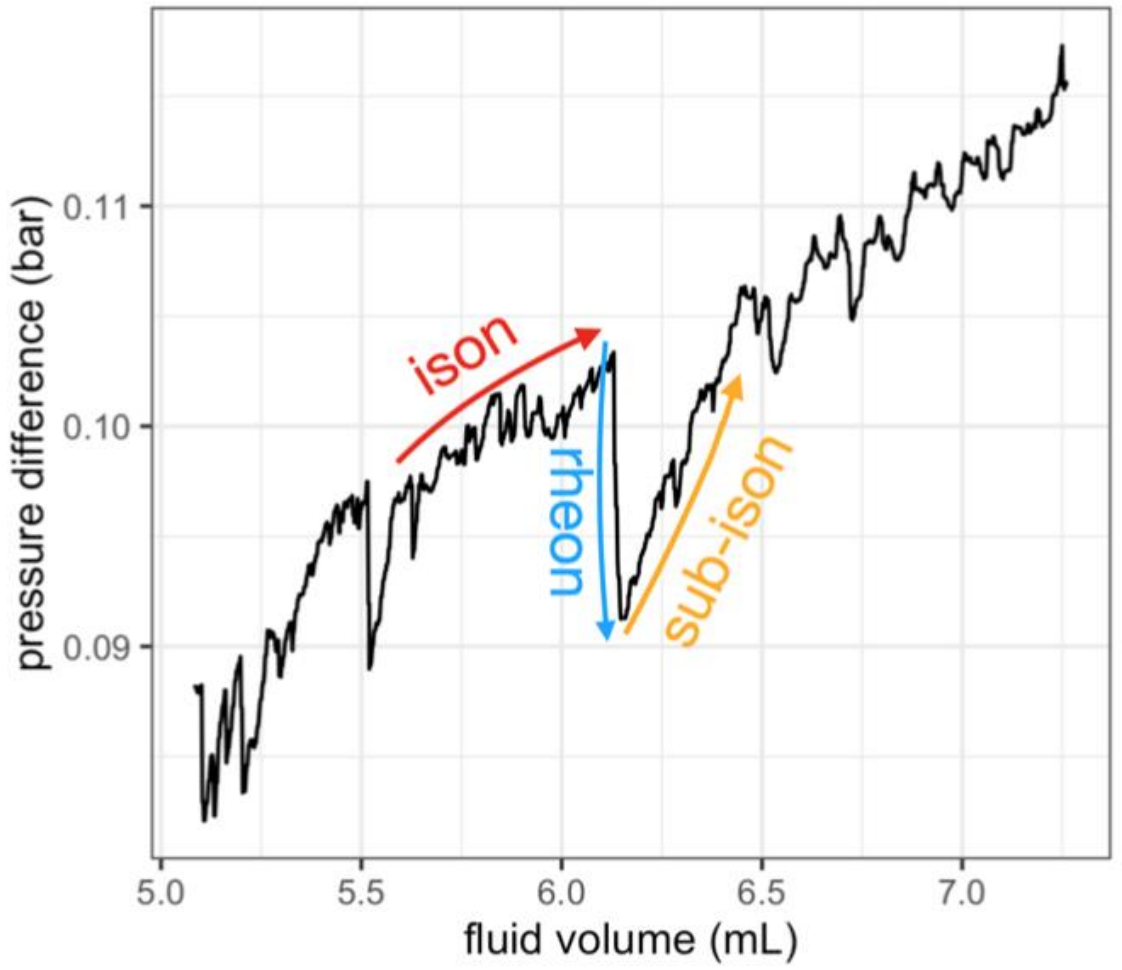
McClure, J.E., Fan. M., Berg, S., Armstrong, R.T., Berg, C.F. Ramstad, T., Relative permeability as a stationary process: energy fluctuations in immiscible displacement. *Physics of Fluids*
(Featured Article) (2022) https://doi.org/10.1063/5.0057428

- Mature digital rock physics simulation capabilities are now in use by industry

McClure, J.E., Li, Z., Berrill, M. *et al.* The LBPM software package for simulating multiphase flow on digital images of porous rocks. *Comput Geosci* **25,** 871–895 (2021). https://doi.org/10.1007/s10596-020-10028-9

Complex Geometry



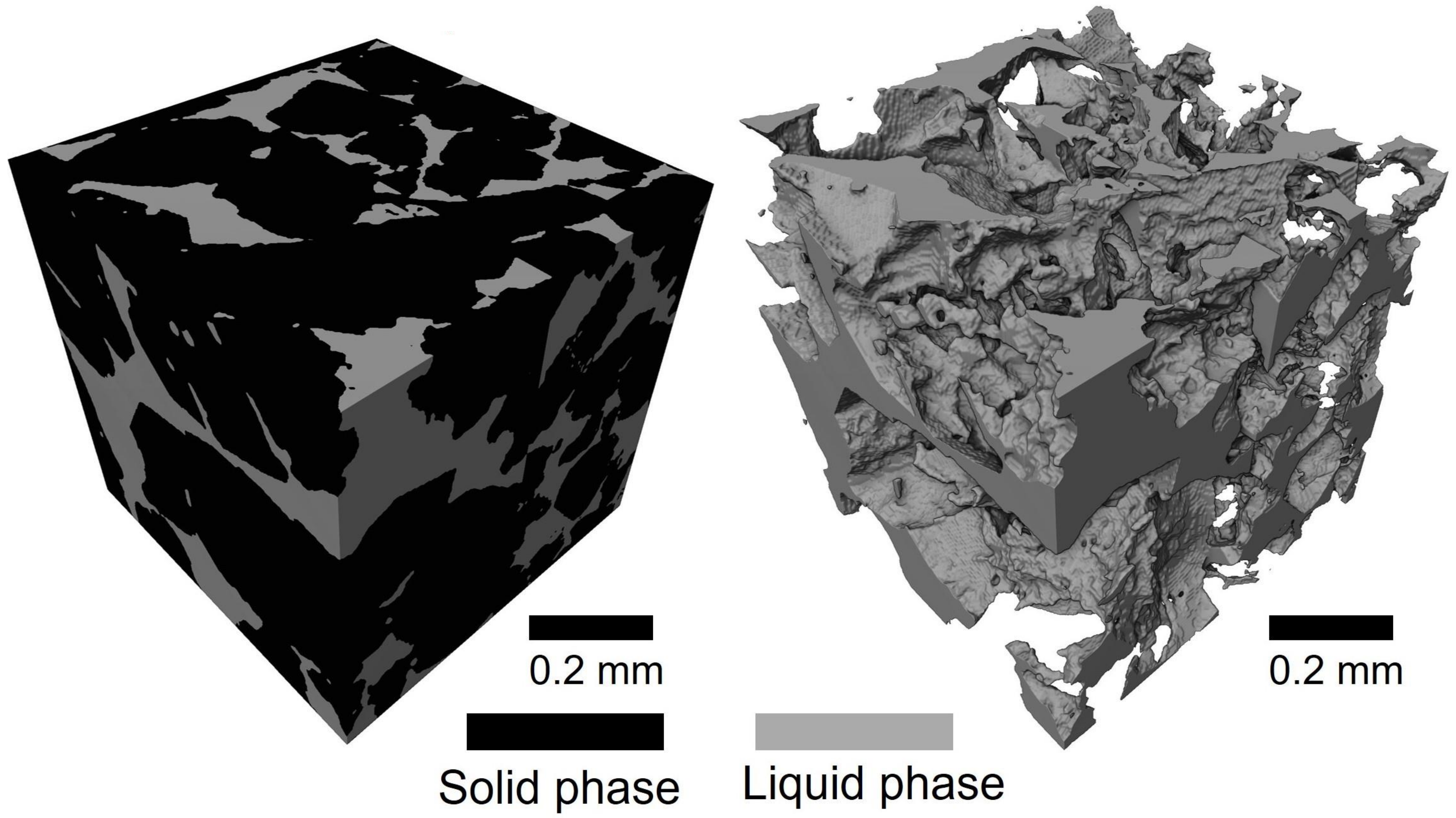


Fluctuating non-equilibrium dynamics

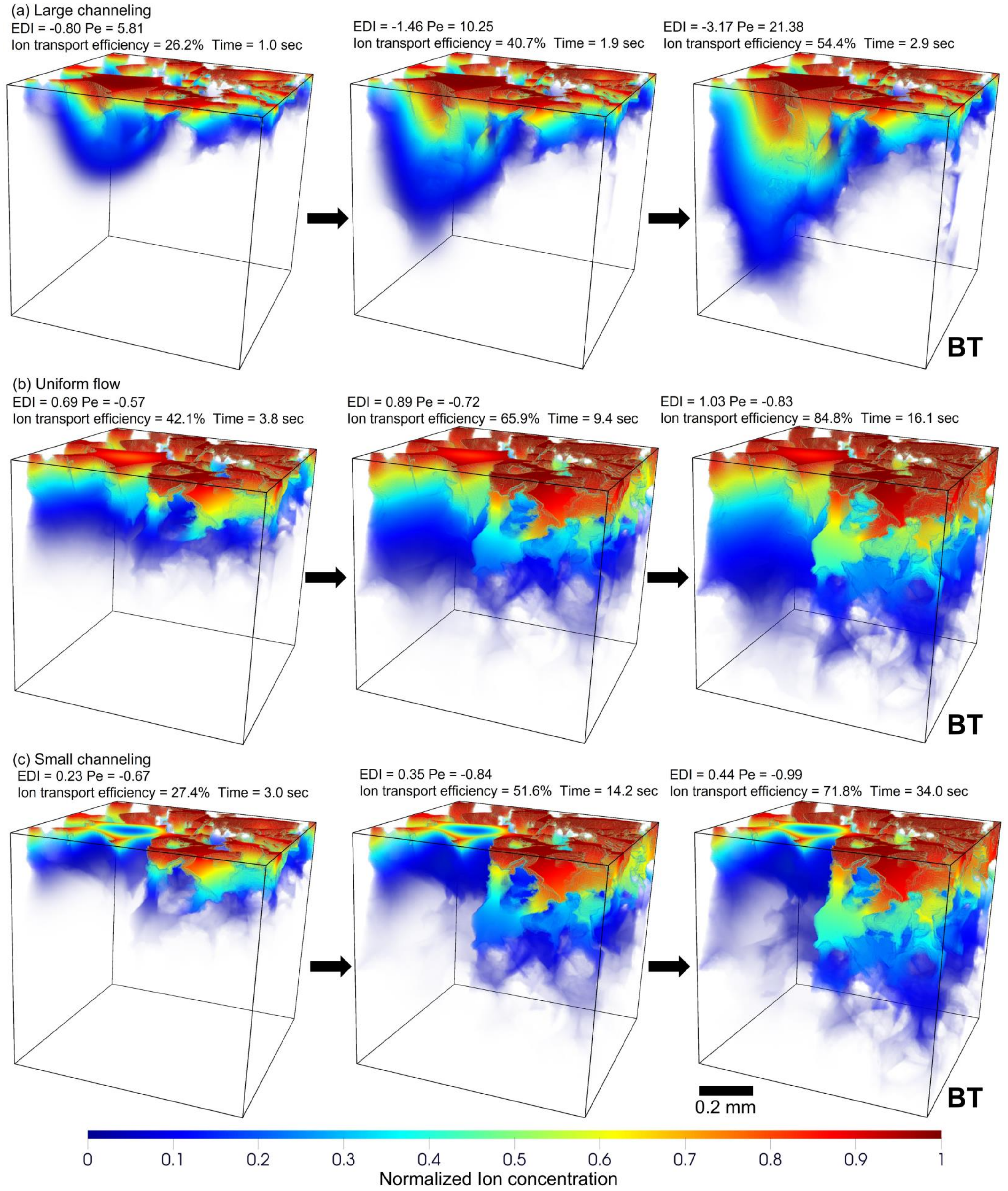
Rare Earth Elements

Ion Transport in Geological Materials

Microscope image data for material structure



Electrical tuning for dominant transport regime

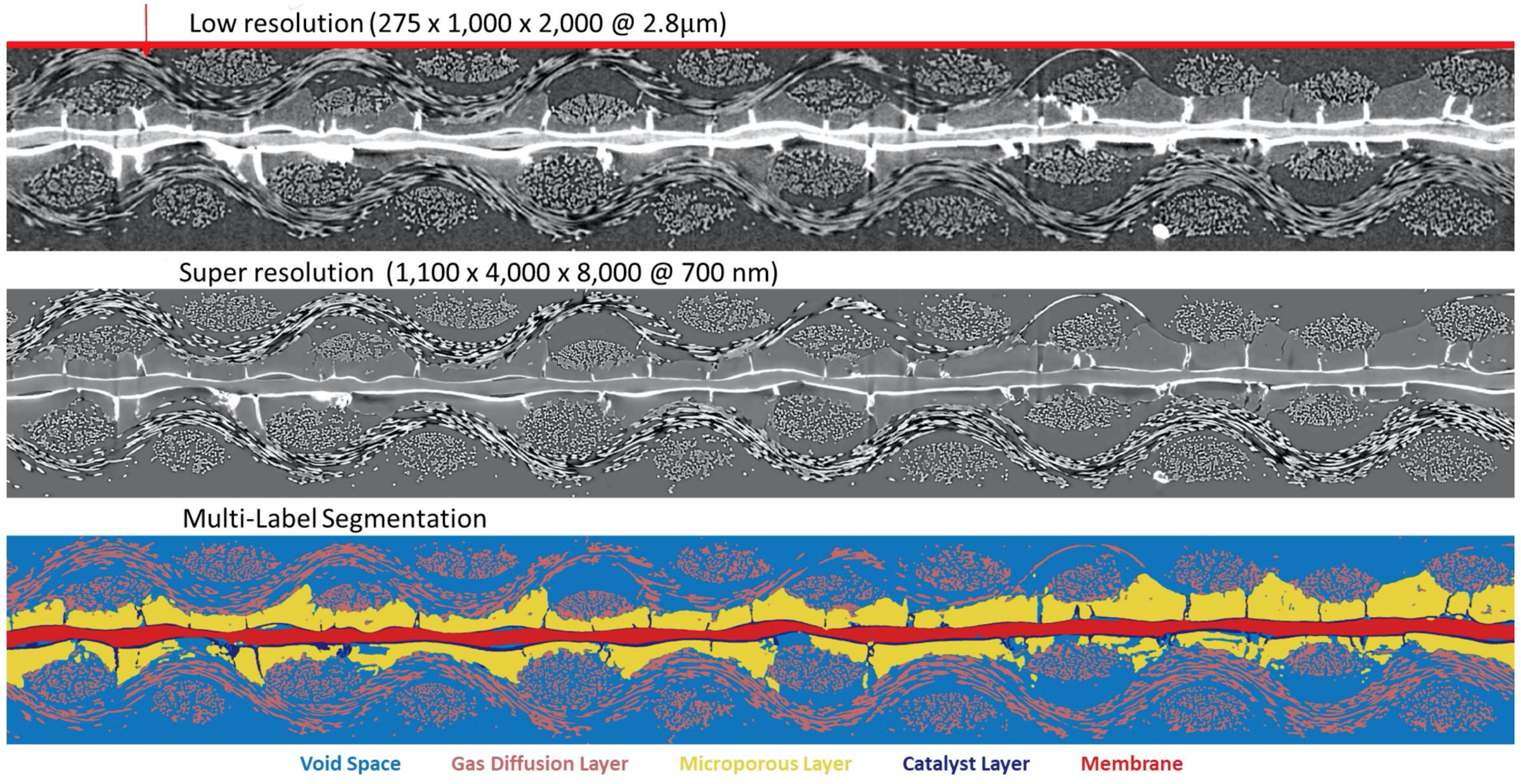


Tang et al. A pore-scale model for electrokinetic in situ recovery of copper: the Influence of mineral occurrence, zeta potential, and electric potential, Transport in Porous Media, 1-26 (2023)
https://doi.org/10.1007/s11242-023-02023-2

Hydrogen Fuel Cells

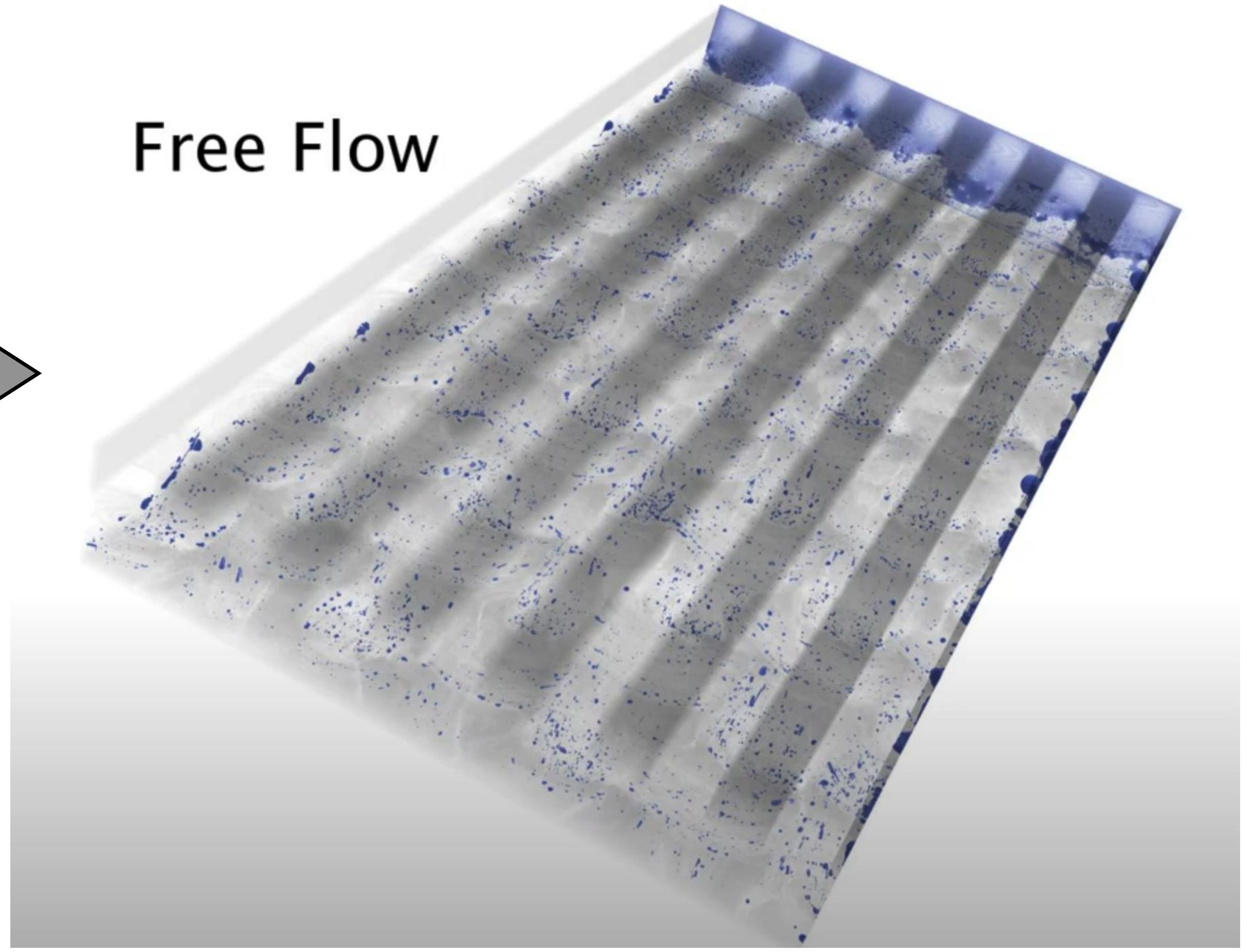
Structural optimization and performance tuning

AI-based super-resolution and segmentation

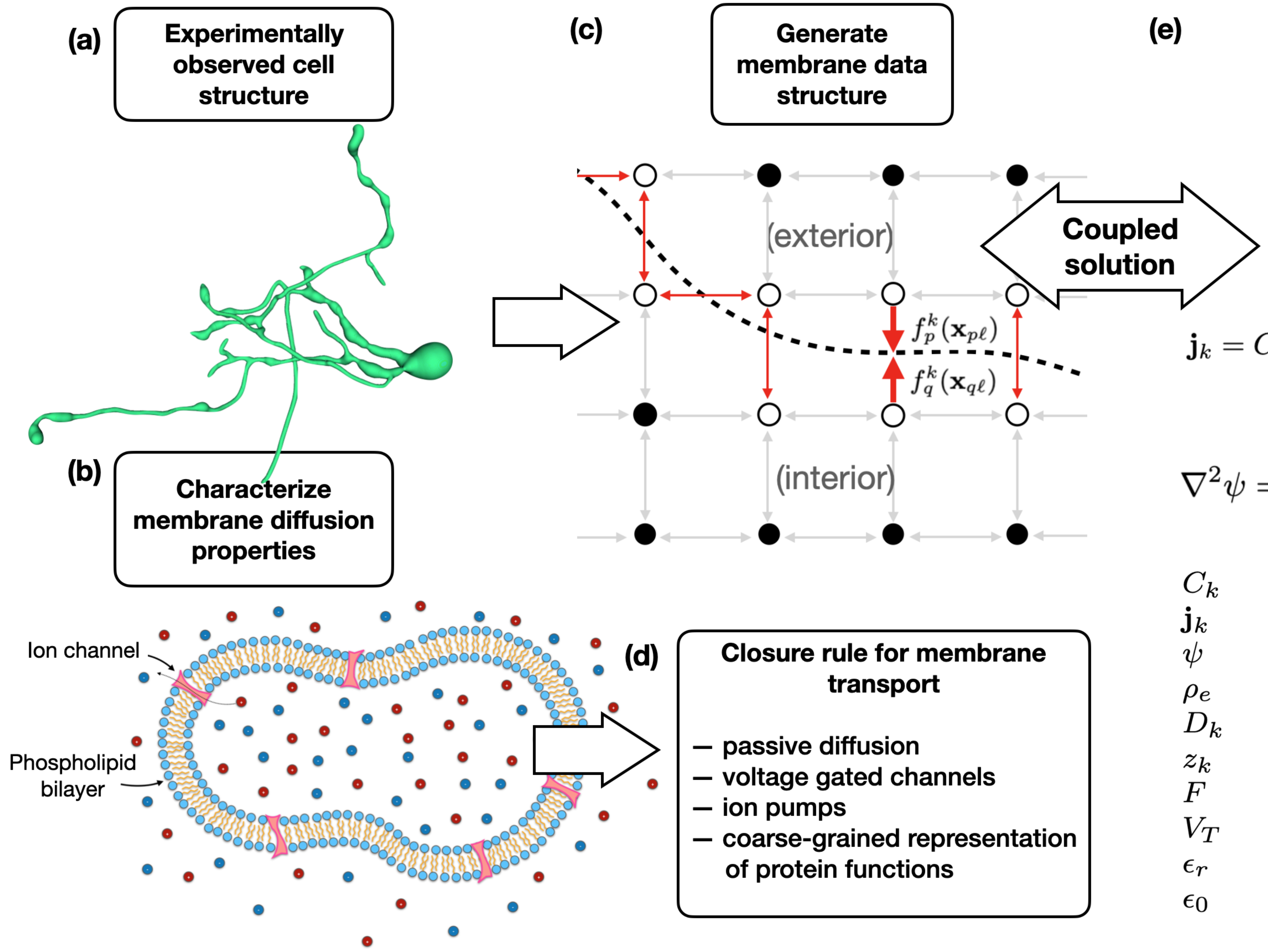


Da Wang et al. Large-scale physically accurate modelling of real proton exchange membrane fuel cell with deep learning. Nature Communications (2023) 14, 745. https://doi.org/10.1038/s41467-023-35973-8

Structural optimization & simulation



Cell Biology — membrane biophysics



(e) **Lattice Boltzmann model for non-equilibrium transport**

Nernst-Planck Equations

$$\frac{\partial C_k}{\partial t} + \nabla \cdot \mathbf{j}_k = 0 \,,$$

$$\mathbf{j}_k = C_k \mathbf{u} + D_k \Big(-\nabla C_k - \frac{z_k C_k}{V_T} \nabla \psi \Big) \,,$$

Gauss's Law

$$\nabla^2 \psi = -\frac{\rho_e}{\epsilon_r \epsilon_0} \,, \qquad \rho_e = \sum_k F z_k C_k$$

C_k	concentration for ion k
$\mathbf{j}_k$	flux for ion k
ψ	electrical potential
ρ_e	charge density
D_k	diffusion coefficient for ion k
z_k	valency for ion k
F	Faraday constant
V_T	thermal voltage
ϵ_r	relative permittivity
ϵ_0	free-space permittivity

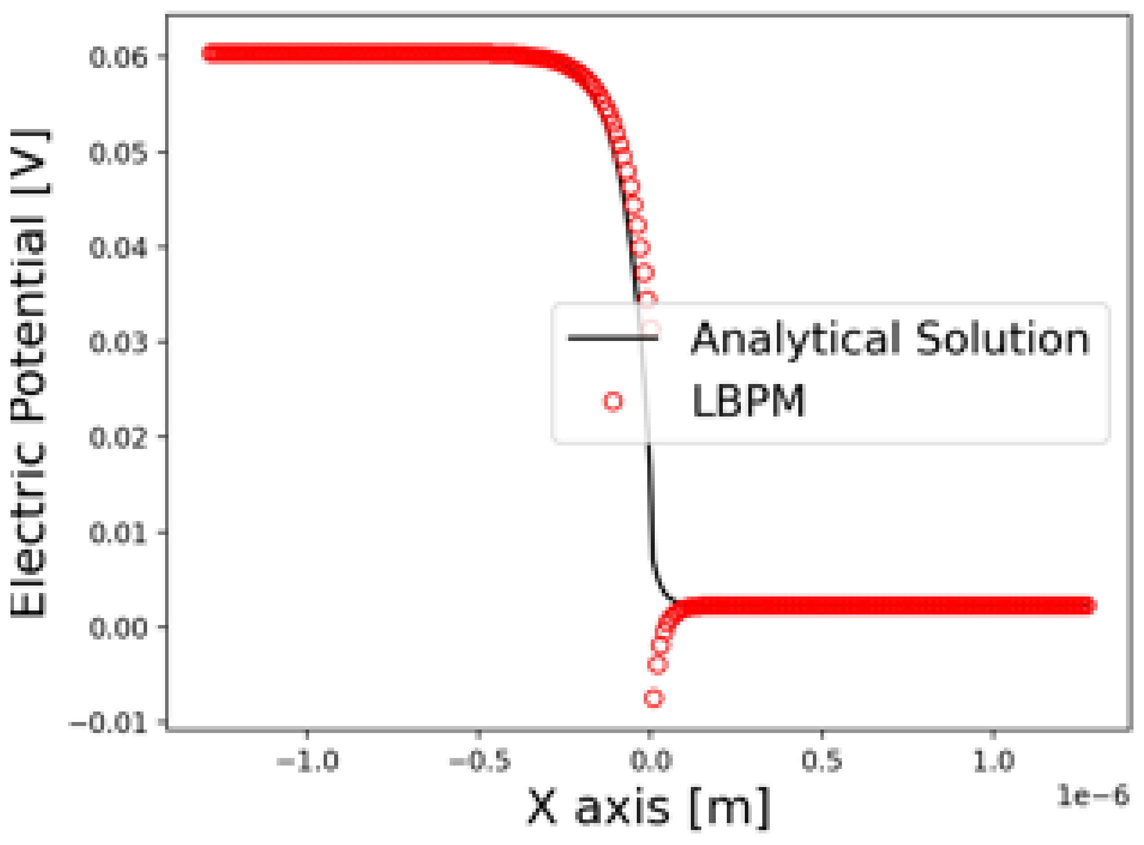
McClure & Li. Capturing membrane structure and function in lattice Boltzmann models, Physical Review E (2023) 107 (2), 024408 https://doi.org/10.1103/PhysRevE.107.024408

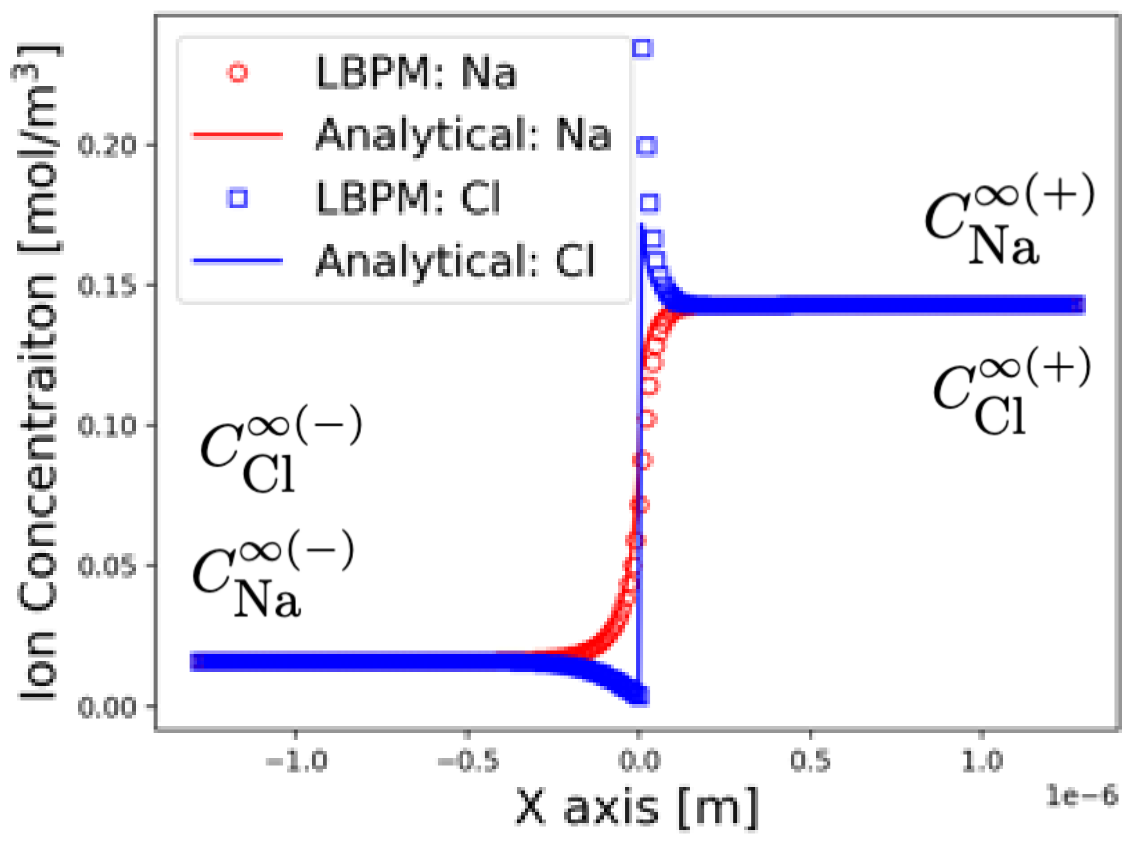
Nernst Potential

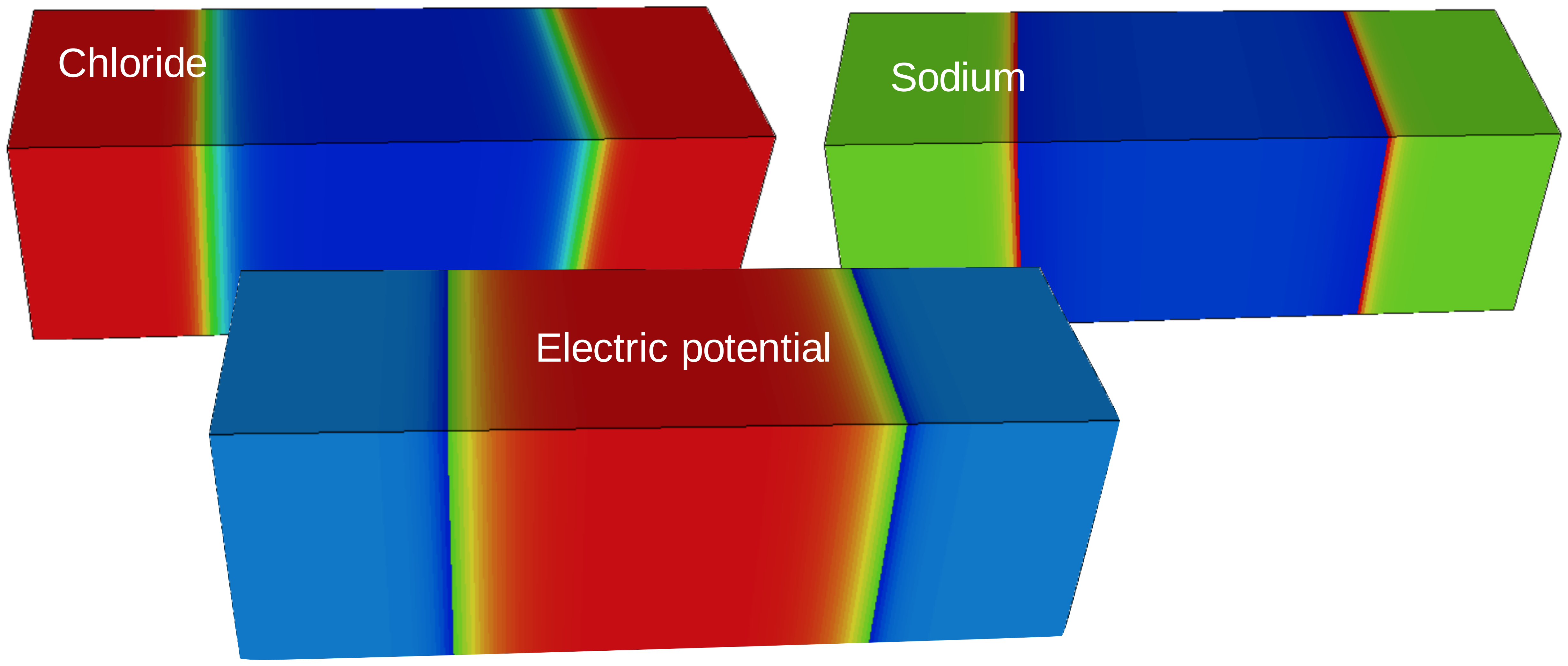
- Predict the electric potential from concentration

$$z_k \frac{\psi^*}{V_T} = \ln \frac{C_k^{*(\text{out})}}{C_k^{*(\text{in})}}$$

- Linearized Poisson-Boltzmann breaks down in vicinity of membrane
- Analytical solution fails to fully capture discontinuity in electric potential (even with non-linear form)
- Membrane charge density should be simulation output (not input)



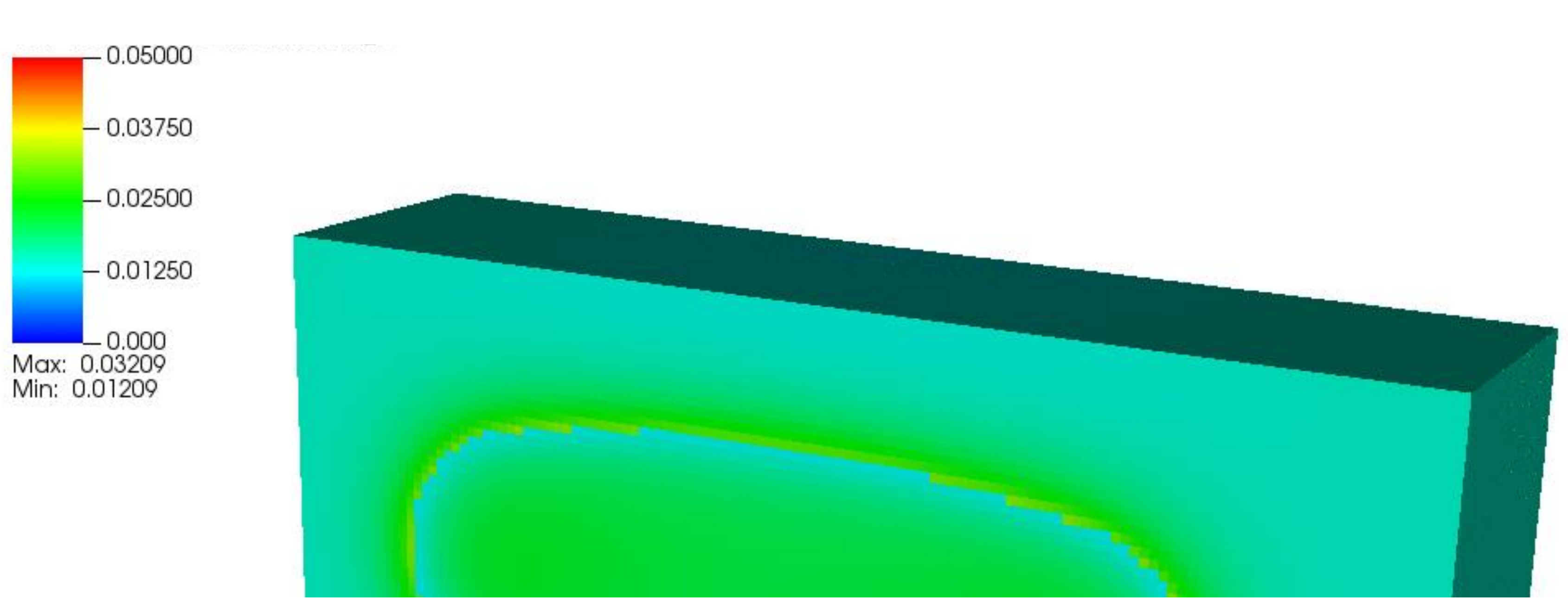


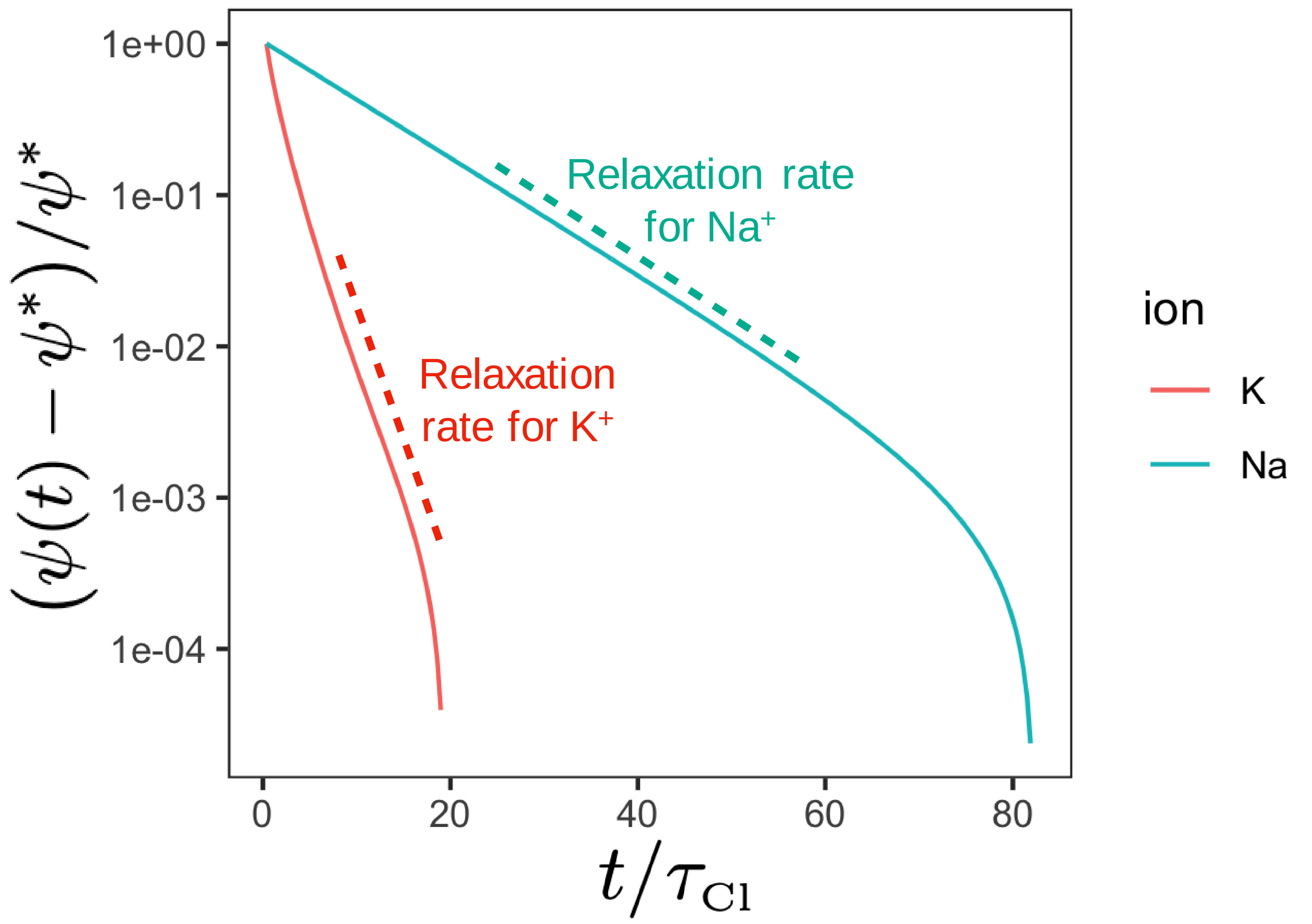


Membrane Charging Dynamics

- Charging dynamics depend on membrane geometry and permeability
- Initial conditions are chosen as follows:
  - gradient in ionic strength
  - electrically neutral on both sides of membrane
  - membrane permeable to one ion at a time
- Transport coefficients can be determined independently for each ion

$$\frac{\psi(t) - \psi^*}{\psi^*} = \exp\left[\frac{t - t_0}{\tau_k}\right]$$





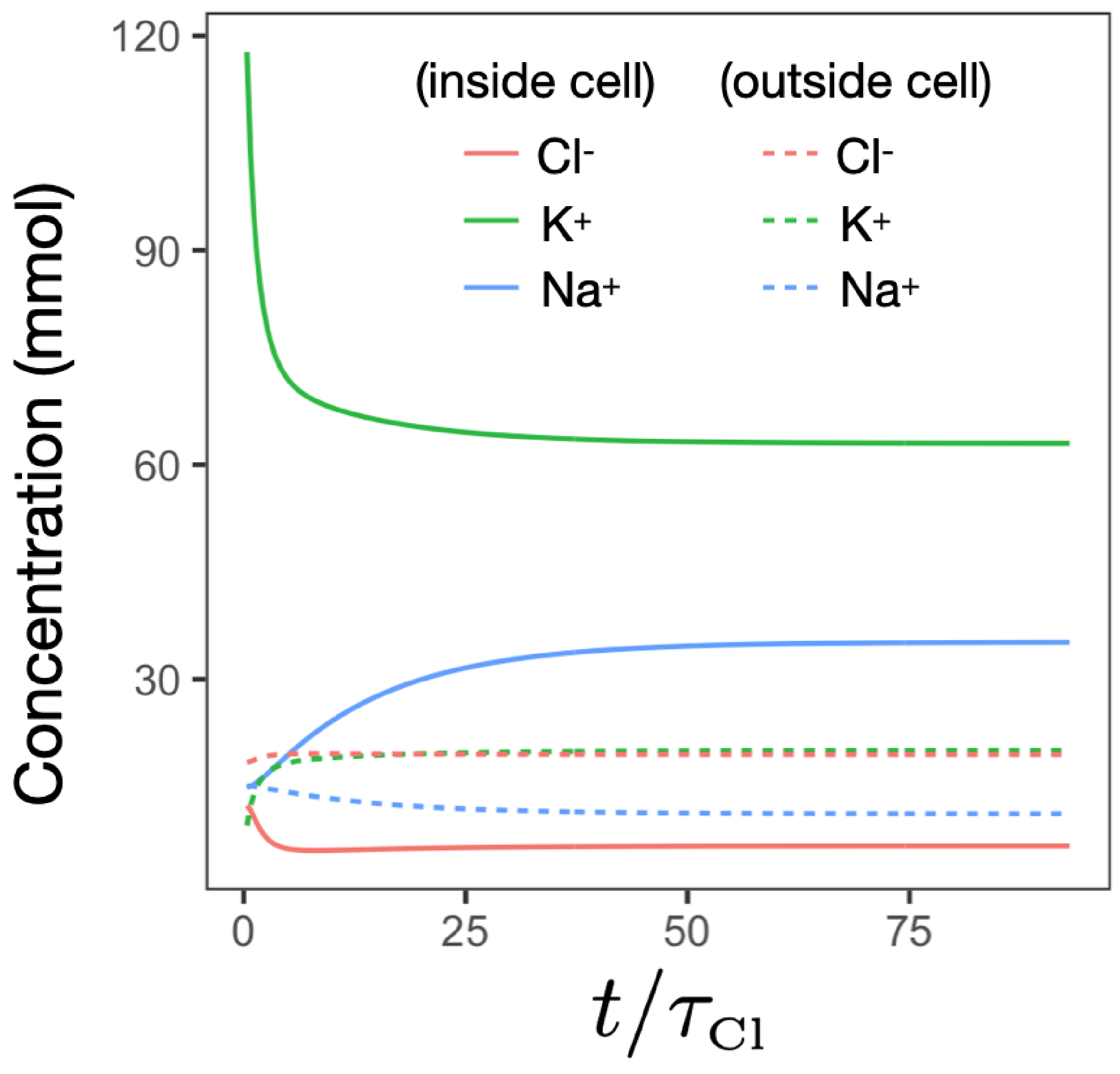
Goldman Potential

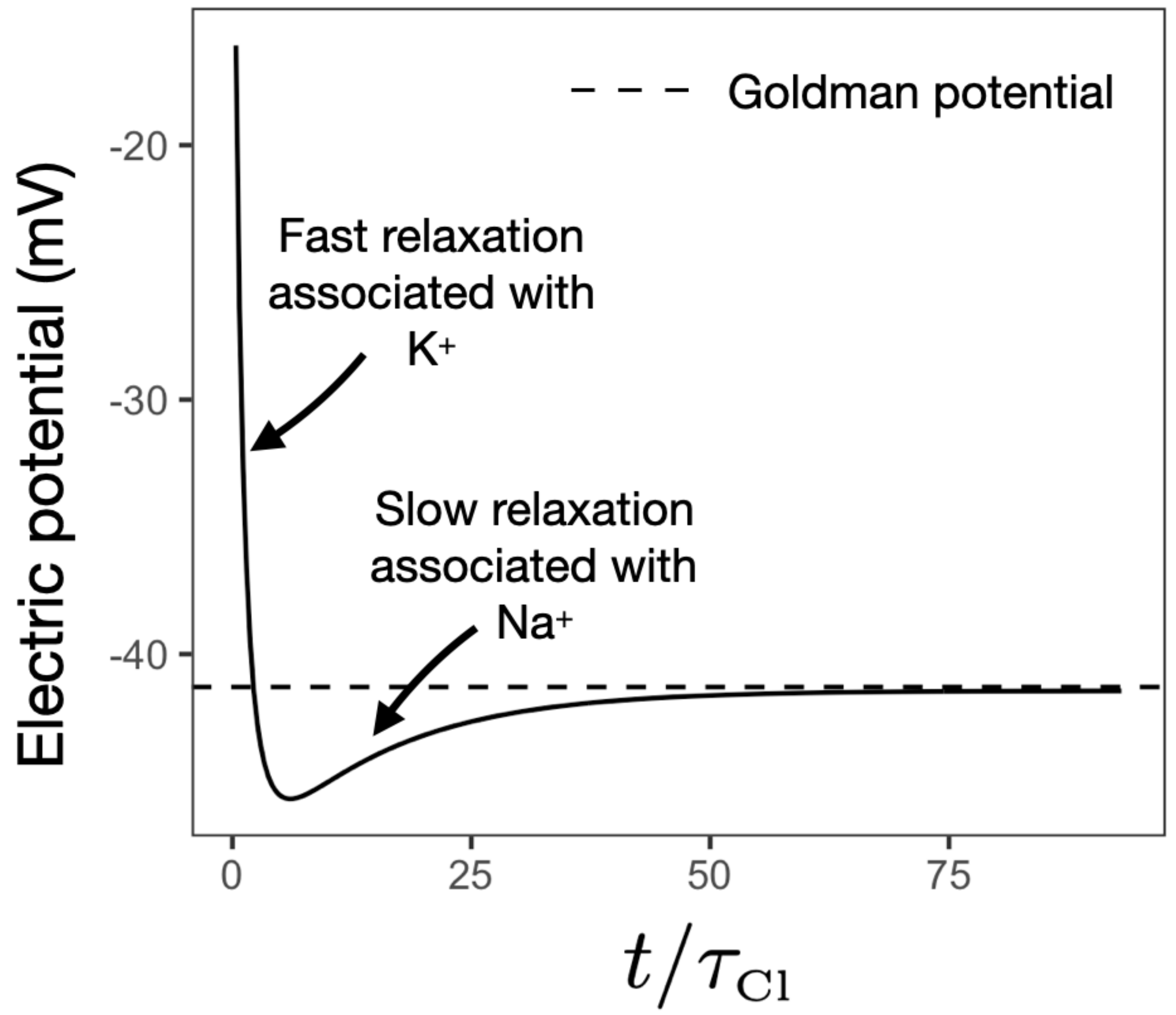
- Membrane permeable to multiple ions

$$\frac{\psi^*}{V_T} = \ln \frac{p_{\mathrm{K}} C_{\mathrm{K}}^{*(\mathrm{out})} + p_{\mathrm{Na}} C_{\mathrm{Na}}^{*(\mathrm{out})} + p_{\mathrm{Cl}} C_{\mathrm{Cl}}^{*(\mathrm{in})}}{p_{\mathrm{K}} C_{\mathrm{K}}^{*(\mathrm{in})} + p_{\mathrm{Na}} C_{\mathrm{Na}}^{*(\mathrm{in})} + p_{\mathrm{Cl}} C_{\mathrm{Cl}}^{*(\mathrm{out})}}$$

- Multiple relaxation timescales produce refactory period for membrane

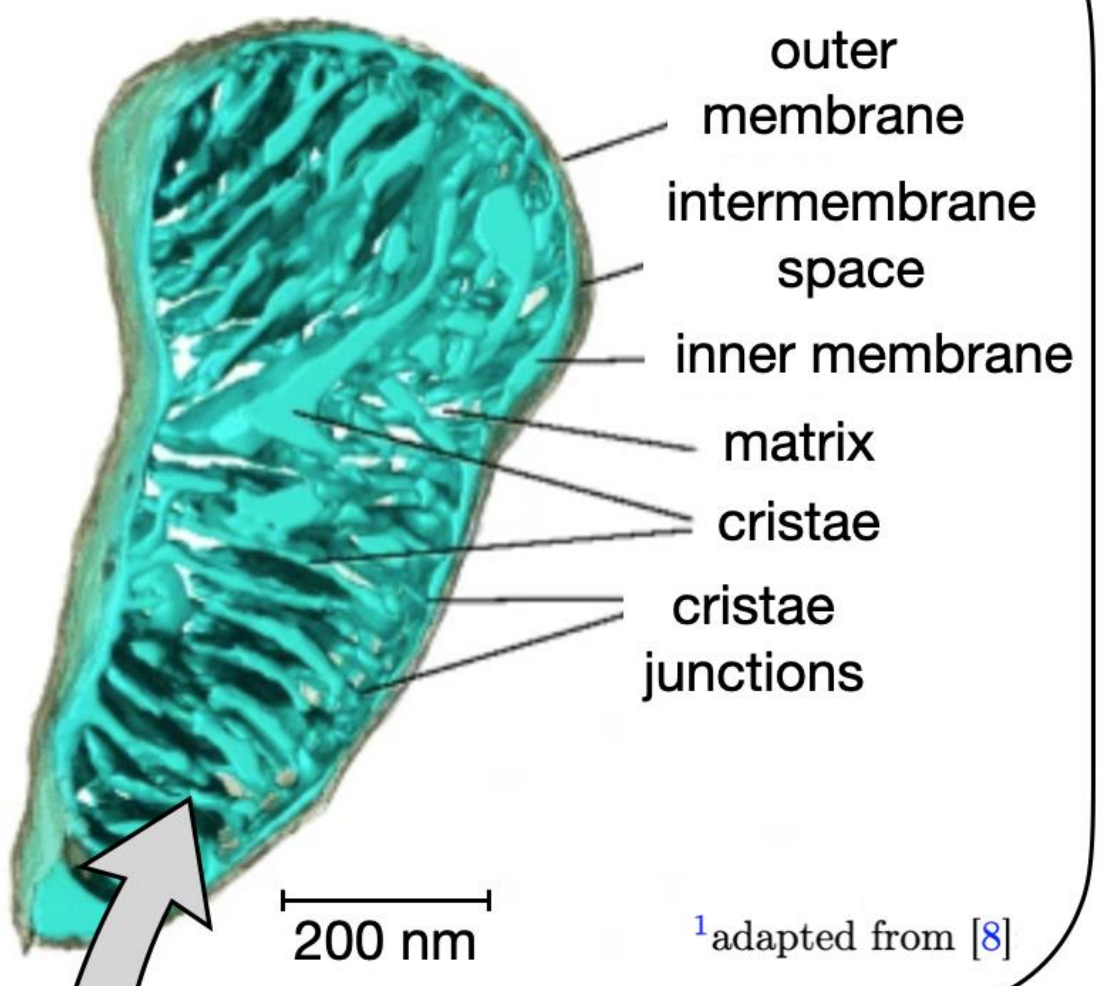
- Cell potential eventually relaxes to the value predicted by Goldman equation (stationary value)





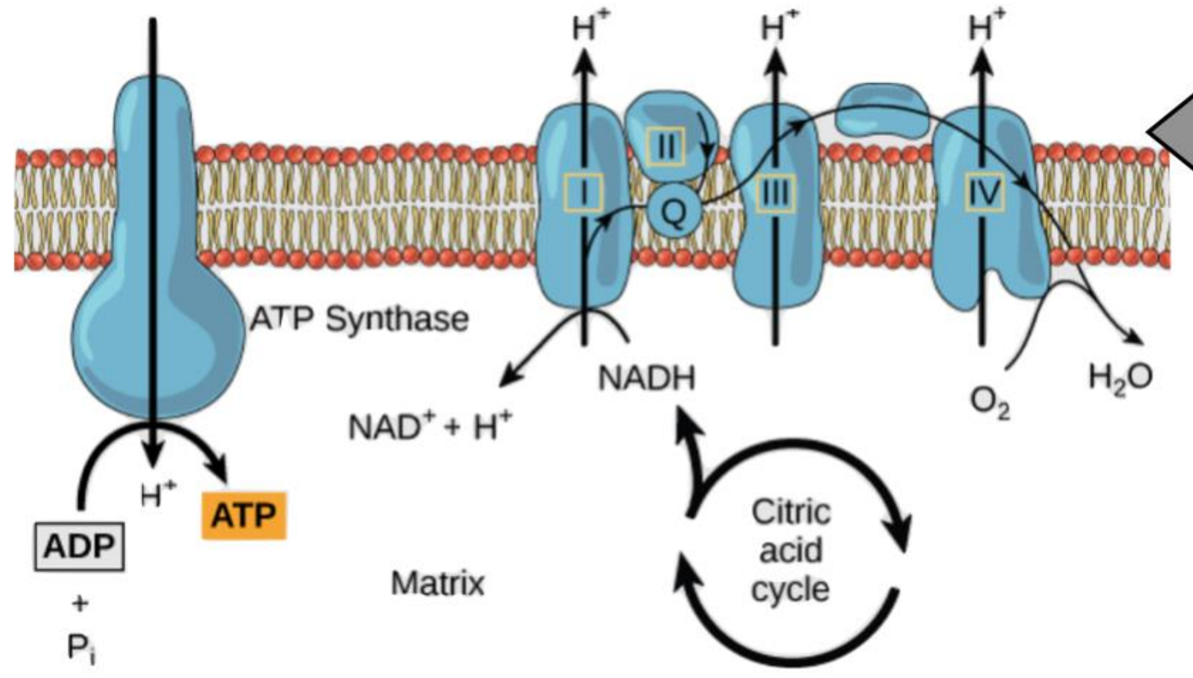
Cell Biophysics — Future Vision

(A) Mitochondria Structure [1]



[1]adapted from [8]

(B) Electron transport chain [2]



[2]adapted from [11]

microscope image data

genomic control of membrane proteins

(C) Coarse-grained representation of ion transport

Effective membrane diffusion properties

Experimental techniques

Molecular dynamics

Mesoscopic Modeling with Lattice Boltzmann Methods

Electronic structure of membrane

- Structure of Guoy-Chapman layer
- Effect of geometry on capacitance
- Losses due to ion leakage

Non-equilibrium responses

- Link membrane transport with overall rate limitations
- Determine thermodynamic efficiency for “cellular engine” from first principles

Characterize behavior and evaluate optimal performance regimes

End Goal — Support laboratory synthesis of new biotechnology capabilities

Next Steps

- **Interfaces for biological systems**— Improve workflows to ingest microscope image data and incorporate AI/ML models to automatically label cell structures
- **Soil microbial community dynamics** — develop enhanced capabilities for systems with complex structure
- **Reactive transport** — Incorporate chemical reactions into the electrochemical modeling framework
- **AI-based closure models**— Develop and validate physics-informed machine learning models to define complex constitutive models (membrane transport, biofilms, chemical reactions)

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OPEN POROUS MEDIA

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